MASTER

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ELECTRON COLLISIONS WITH POSITIVE IONS

Progress Report

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ABSTRACT

Collision strengths for electron impact excitation of the 2s-2p, 2s-3s, and 2p-3s doublets of Li-like O^{5+} were calculated for energies between the 3s and 3p levels, and for excitation of the 2s-2p, 2s-3s, 2s-3p, and 2p-3p doublets for energies between the 3p and 3d levels. Calculations were made in a five-state close-coupling approximation. Autoionization resonances in the scattering collision strengths were included through quantum defect theory analysis. Resonance contributions enhanced the allowed 2p-3s collision strength by factors of 6.8 and 2.8 in the energy regions, respectively. The forbidden 2s-3s collision strength is enhanced by lesser amounts, by factors of 2.0 and 1.2, respectively. Collision strengths were calculated for Zn^+ from the 4s ground state to excited states 4p, $3d^9\ 4s^2$, 5s, and 4d in a five-state close-coupling approximation for the electron impact energy range $15 < E < 400$ eV. Very good agreement with measurements of absolute emission cross sections of Rogers et al. was obtained for the energy range $15 < E < 100$ eV, when cascade contributions were included. A two-state close-coupling approximation was used to calculate inner-shell excitation of Zn^+ for transitions $3d^{10}\ 4s \rightarrow 3d^9\ 4s5\ell$. These excitation-autoionization processes were shown to enhance by factor of two, the ionization cross section for Zn^+ in the energy region up to five times the ionization threshold.

This progress report concerns a program of computation of collision strengths for the electron impact excitation of ions. The report covers the first year of contract No. DE-AS05-80ER10609 from April 1, 1980 to March 31, 1981.

The effect of resonances on lithium-like O^{5+} at energies below the 3d state has been calculated.[1] A close-coupling expansion including the 2s, 2p, 3s, 3p, and 3d states of the ion is employed. Each state is represented by a Hartree-Fock wave function. The calculation uses a non-iterative integral equation method (NIEM) of Smith and Henry[2] to solve the coupled integro-differential equations which arise in the close-coupling expansion. Calculations are made at a number of energies above the 3d state and program RANAL[3] is used to obtain the detailed and averaged collision strengths. This program uses quantum defect theory[4] to analyze the reactance matrix elements. Direct calculations made in the resonance region for one partial wave confirm the position and width of the resonances obtained with RANAL. Resonance contribution to collision strengths enhances the allowed 2p-3s and forbidden 2s-3s values by factors of 6.8 and 2.0 in the energy region below the 3p state. Between the 3p and 3d states, the resonance enhancement is 2.8 and 1.2, respectively. The average effect of resonance contributions to $\Omega(2s,2p)$ is found to be only 4%. The resonance effects depend on the strength of coupling to a closed channel, which it is conjectured may be gauged by considering collision strengths for energies such that all channels are energetically accessible.

Inelastic electron impact collision strengths have been calculated[5] for Zn^+ from the 4s ground state to excited states 4p,

$3d^9\ 4s^2$, 5s, and 4d in a five-state close-coupling approximation for the electron impact energy range $15 < E < 400$ eV. Each state is represented by Hartree-Fock functions except for the excited $^2P^o$ state which is given by a three configuration function. The calculations use an NIEM method.[2] Very good agreement with measurements of absolute emission cross sections of Rogers et al.[6] is obtained for the energy range $15 < E < 100$ ev, when cascade contributions are included. Poorer agreement is obtained with experiment for excitation of the 5s state, due to sensitivities in the close-coupling approximation.

A significant contribution to electron impact ionization of Zn^+ comes from an excitation-autoionization process. In it, an inner-shell electron is excited and subsequently loses its energy by the ejection of a more loosely bound electron from an outer shell. If all of the excited states autoionize then the total ionization cross section is obtained by adding the sum of inner-shell excitation cross sections to the direct knock-on ionization cross section. A two-state close-coupling approximation was used to calculate[7] inner-shell excitation of Zn^+ for transitions $3d^{10}\ 4s \rightarrow 3d^9\ 4s5\ell$. The excited states considered were $^2P^o$, $^4P^o$, $^4F^o$, $^2D^o$, ^2P, and ^2D. Excitation-autoionization contributions to the total ionization cross section are found to exceed the direct ionization contribution for the energy region $22 < E < 100$ eV. This enhancement is in very good qualitative agreement with experiment.[7]

The work currently in progress, which will be continued during the remaining four months of this contract year, can be summarized as follows:

1. The effect of resonances in the closed channel region is being obtained for lithium-like carbon, neon, and argon. Thus, when incorporated with our results for O^{5+}, we will be able to obtain the resonance effects as a function of atomic number for the lithium isoelectronic sequence. Then we can predict its importance for Cr, Fe, Ni, and Ti.

2. Development of iterative exchange methods and other computer programs will continue.

During the current contract year, Dr. Henry spent 12.5% of his time during the academic year and 33.3% of his time for 3 months in the summer working on this contract. Dr. K. Bhadra, a post-doctoral research associate, spent 100% of his time each month on this contract from its inception on April 1, 1980.

REFERENCES

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ARTICLES PREPARED FOR PUBLICATION IN CONTRACT YEAR 4/80-3/81

ORO-10609-01 Effect of Resonances on 2s-2p and $2\ell-3\ell'$ Excitation of O^{5+} by Electron Impact.
K. Bhadra and R. J. W. Henry
Phys. Rev. Letts. (submitted)

ORO-10609-03 Electron Impact Excitation of ZnII
A. Z. Msezane and R. J. W. Henry
Phys. Rev. A (to be submitted)

ORO-10609-04 Electron-Impact Ionization of Zn^+ and Ga^+
W. T. Rogers, G. Stefani, R. Camilloni, G. H. Dunn, A. Z. Msezane, and R. J. W. Henry
Phys. Rev. A (to be submitted)